

RANDOM TILING TRANSITION IN THREE DIMENSIONS

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Three-dimensional icosahedral random tilings are studied in the semi-entropic model. We introduce a global energy measure defined by the variance of the quasi-lattice points in orthogonal space. The specific heat shows a pronounced SCHOTTKY type anomaly, but it does not diverge with sample size. The flip susceptibility as defined by Dotera and Steinhardt [Phys. Rev. Lett. **72**, 1670 (1994)] diverges and shifts to lower temperatures, thus indicating a transition at $T = 0$. Contrary to the Kalugin-Katz conjecture, the self-diffusion shows a plateau at intermediate temperature ranges which is explained by energy barriers and a changing number of flipable configurations.

1 Introduction

The stability of quasicrystals has been a subject of intensive research since they were discovered in 1984. In the random tiling (rt) model stability is ascribed to the entropy S . If the internal energy U also contributes one is dealing with the semi-entropic model characterized by a free energy $F(T) = U(T) - TS(T)$. The rt model is an abstraction where tiles cover the whole space without gaps. Thermal fluctuations and deformations of the tiles and phonon degrees of freedom are neglected. The only dynamic motion that exists is a local rearrangement of tiles, called “flips”.

2 Random tiling characterization

A random tiling may be characterized by the mean square deviation of the point distribution from the center of mass in the orthogonal space. The variance is defined by $\Omega = \overline{\mathbf{y}^2} - \bar{\mathbf{y}}^2$ (1), where the average is over all vertices N , and \mathbf{y}_i are the position vectors in orthogonal space. The lattice points of a quasicrystal are distinguished by their local environments. There are 24 allowed vertices, but 5450 vertices may occur in a random tiling. In the icosahedral rhombohedron tiling some flips change only the frequency of vertices without introducing forbidden vertices. But if the degree of randomization has reached a certain level the number of forbidden vertices starts to rise rapidly. The rhombohedron tiling contains dodecahedra enclosing two prolate and two oblate rhombohedra. The internal vertices are called simpletons and are arranged in two-dimensional layers perpendicular to two-fold symmetry axis. A spin can be assigned to the simpletons² depending on their position. In the ideal tiling all the spins in

a certain layer carry spin +1 or -1. With a proper summation rule a sheet magnetization M of value 1 is formed. In a random tiling the sheets exist with a reduced value since the spins are no longer aligned. The susceptibility is given by $\chi = 1/T < N_D > (< M^2/N_D^2 > - < M/N_D >^2)$, N_D is the number of spins.

3 Energy measures

In this work we deal with canonical rt ensembles. All configurations of one ensemble have the same volume and the same number of particles. The pure entropic rt model, on the other hand, is specialized for microcanonical ensembles, since all configurations have the same energy. Starting from a canonical rt ensemble in the thermodynamic equilibrium we can calculate the internal energy as the ensemble average $U = \langle E \rangle$ of the instantaneous energy E . The specific heat $C_V(T)$ may then be derived from the variance $< (\delta E)^2 >$. The entropy density $s(T)$ ^a is given by the integration of the specific heat c_V . The ground state entropy s_0 represents the number of states energetically equivalent to the quasiperiodic ground state. At $T \rightarrow \infty$ we are in the limit of the pure rt model and we get the configuration entropy s_∞ . The temperature variation of the c_V depends on the energy measure, but s_∞ is independent of it. This is especially the case if the following holds: First, the energy of any configuration is unique. Second, the quasiperiodic reference tiling is a ground state. For global energy measures states with an energy less than the quasiperiodic reference tiling may exist which would indicate that this state is not stable at $T = 0$. Third, the energy measure is limited from above. This is a requirement for the integrability of $c_V(T)/T$ as a function of T . If the energy measure is not limited, uncontrolled fluctuations of the energy in the high-temperature limit may exist. If they vary stronger than quadratic with T then $< (\delta E)^2 > / T^2$ diverges together with c_V as $T \rightarrow \infty$.

A globally defined energy measure with easily calculable ground state entropy is the “harmonic energy measure”. The energy is given by the sum of the squared distances of the dual quasilattice sites from their center of mass. Up to a factor N it is equal to the variance Ω in the orthogonal space. The energy of the configuration α is given by $E^{(\alpha)} = CN|\Omega^{(\alpha)} - \Omega^{(0)}|$ (2). The index 0 denotes the ideal reference configuration, C is a normalization constant. The variance for the ideal reference configuration 0 is smaller than the variances for the overwhelming majority of the rt configurations α . But there is a tiny minority of configurations with a variance smaller than the value of the ideal tiling. Their atomic hypersurfaces are closer to a sphere than the triacon-

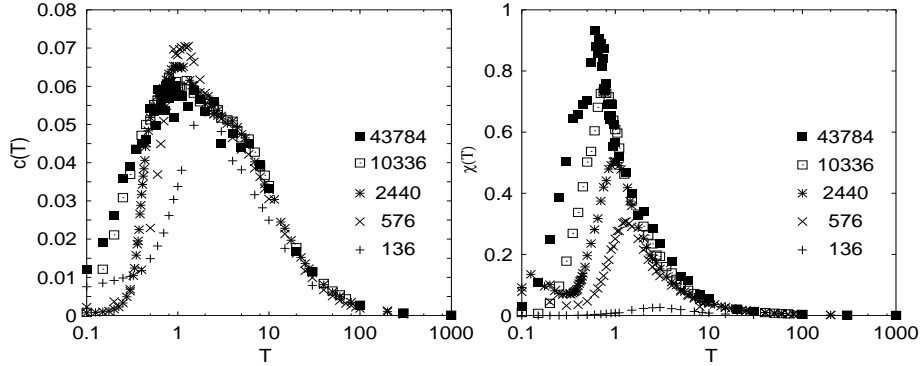
^aLarge letters indicate total quantities, small letters denote quantities per tile.

tahedron. To avoid energies less than the energy of the ideal tiling we have taken the absolute value in Eq.2. For zero global phason strain this energy measure is not degenerate. But for periodic approximants the N possibilities to chose the origin of the unit cell yield a ground state entropy $s_0 = \ln N/N$ per lattice point which vanishes in the thermodynamic limit. Strandburg³ has introduced a similar energy measure. But it was taken relative to a fixed point in the orthogonal space and not relative to the center of mass and therefore does not fulfil the criterium of finiteness of the energy measure. Without fixed boundaries of the system the whole distribution of vertex points in orthogonal space may drift and therefore yield a systematic contribution to the energy.

4 Results

A plot of the c_V and χ vs. T for different sample sizes (finite-size scaling) may disclose a second order phase transition if it diverges with sample size. To prove this, ensemble averages were calculated for five cubic approximants from 136 ($n = 3$), up to 43784 ($n = 7$) vertices (n is the generation). The internal energy grows monotonously but saturates at $T \rightarrow \infty$ at a value depending on the size of the sample. The limit can be derived from limits of the variance: $\Omega(T = \infty) = 1.73 \pm 0.01$ and leads to u between 1.97 and 2.05. A SCHOTTKY anomaly is present in the c_V -plot (Fig. 1) but the specific heat shows an additional bump above the maximum. Such a behaviour is known for few-level systems with sufficiently separated levels. We have mapped the distribution of the energy levels for $T = \infty$. No indication of discrete energy levels was found, only an asymmetry of the distribution with a smaller slope at higher energies was observed. There exist other energy measures¹ which exhibit no visible asymmetry in the energy distribution and no bump in the specific heat. The value of the maximum of c_V is not significantly dependent on sample size. The increase in s_∞ is caused only by the growing width of the maximum. The reason why there is no divergence of the maximum of c_V may be that the intrinsic divergence of the specific heat with sample size, if any, is very weak. For closer insight we calculated the sheet magnetization M and the susceptibility χ since the latter shows a much more pronounced divergence behaviour². The value of the maximum of the susceptibility (Fig. 1) grows about linearly with the generation n and moves to lower T . It is not yet clear if the relation $\chi_{max}(n) \propto (n - n_0)$ is valid for $n > 7$. If yes, this would be a slow divergence (more precisely: $\chi_{max}(N)$ is about proportional to $N^{4.25}$, thus indicating a transition at $T = 0$). The alternation condition² yields much clearer results for c_V and χ — maybe as a consequence of its closer similarity to an Ising model.

Figure 1: Specific heat c and susceptibility χ . Sizes are indicated by the number of vertices.



The mean square displacement grows linearly with time t , indicating a normal diffusion behaviour. The diffusion coefficient forms a plateau at $T > 1$ for $n = 4, 5, 6$ in the ARRHENIUS plot. There may be several reasons for this behaviour: First, there are energy barriers which at low temperatures lower the mobility of lattice points for higher energy flips. In the range of the plateau the probability for a flip only occasionally suffices to overcome the barriers which play no role at high temperatures. Second, a phase transition may exist which changes the slope in the ARRHENIUS plot. This is how Gähler explained a similar behaviour for the alternation condition. At last, the number of flipable lattice points may change with temperature. The number of simpletons is about 23% in the range $0 < T < 1$. It decreases up to $T \approx 10$. The plateau of $D(T)$ is most clearly seen in this range. Up to $T \approx 100$ the further decline leads to an increase of the negative slope of $D(T)$. Above $T \approx 100$ the number of simpletons is constant at $\approx 17.5\%$. The behaviour of $D(T)$ is obscured to some degree by modes with zero energy cost caused by periodic boundaries. These modes become less important at larger sizes, but they suppress the plateau for small sample sizes.

References

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